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Functionalized Heterofullerenes for Hydrogen Storage PURU JENA, QIAN WANG, Virginia Commonwealth University, QIANG SUN, Peking University and Virginia Commonwealth University — Using density functional theory we show that Li decorated B doped heterofullerene (Li12C48B12) has the desired properties of a hydrogen storage material: (1) The Li atoms remain isolated. (2) Through charge transfer to electron deficient C48B12 heterofullerene, the Li atoms become positively charged. (3) Each Li atom is able to bind up to three H2 molecules which remain in molecular form, and the binding energies of successive H2 molecules are in the range of 0.135 to 0.172 eV/H2, suitable for ambient temperature storage; (4) The gravimetric density reaches the 9 wt % limit necessary for applications in the mobile industry.

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